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Title: An Integrated Approach to HE Product Equation-of-State

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An Integrated Approach to HE Product Equation-of-State*

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LANL High Explosives Review Meeting August 8, 2001

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Introduction

Goal: develop an integrated, practical, and accurate methodology for determining HE product EOS.

Three Elements:

I: Experiment

- Necessary: test(s) for which a useful portion of the product EOS (the wider the pressure range the better) can be uniquely inferred from the measurement.
- **Better:** test(s) for which the *inverse* problem can be *explicitly* computed to infer the governing EOS.

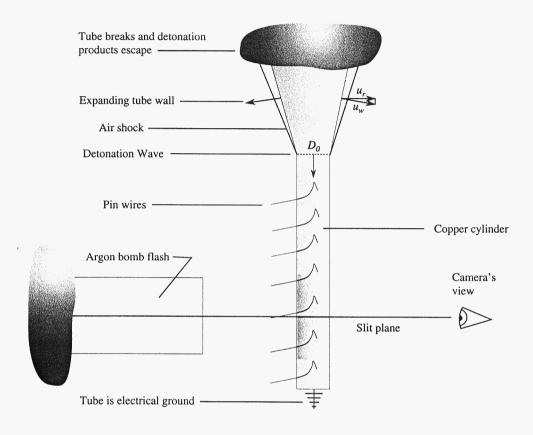
II: Analysis

• Whether one computes the inverse problem, or the (iterative) forward problem: goal is to compute the EOS structure from the data. Historically (i.e. JWL) one asks how well an assumed empirical form flux data.

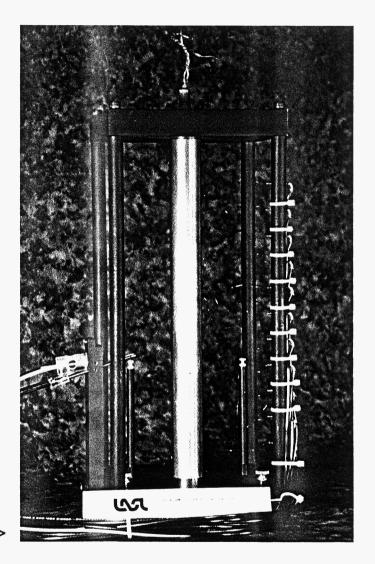
III: EOS Form

- * Use explicit ECS predictions to generate tabular EOS or new, better analytic forms.
- Validation by hydrocode: Do we get the right answer in a variety of configurations?

Schematic of Traditional Cylinder Test



Current Implementation with simultaneous streak camera VISAR, framing camera, velocity pins ----->

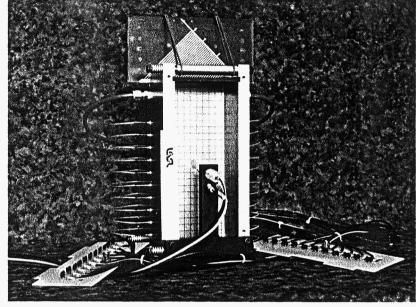


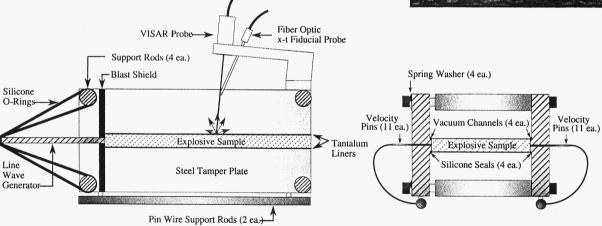
Experiment: Sandwich Test

• The Sandwich test is a recently developed slab variant of the cylinder test that is more datadriven at high pressures, and which also extends to low pressures (~500 Bar).

Photograph of Sandwich Test ---->

Schematic Drawing of Sandwich Test





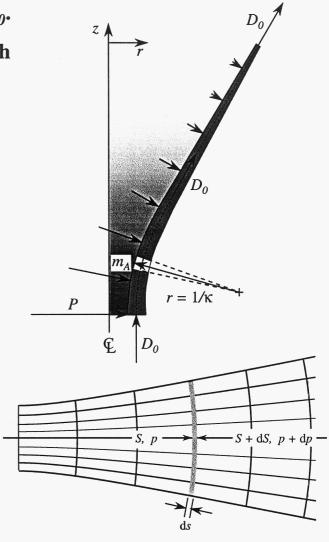
See design details in APS01 Proceedings

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Analysis: Overview of Taylor's Inverse Isentrope Problem

- 1. Determine case shape R(z) from measured R(t) and D_0 .
- 2. Fit a curve to the wall trajectory that is consistent with the model assumptions (strictly incompressible wall).
- 3. Calculate inner contour knowing wall thickness and (in the case of cylinder test) how the tube stretches.
- 4. Calculate wall P(z) using inner contour trajectory. Fundamental observation: wall pressure is proportional to wall trajectory curvature.
- 5. Geometric assumption about pressure iso-contours: relationship between measured wall pressure and internal pressure. Quasi-conical approximation.
- 6. Solve ODE for specific volume v(z), given P(z), from mass and momentum conservation equations.
- 7. Obtain the principal isentrope by plotting P(z) vs. v(z) parametrically.
- 8. Determine the internal energy along the isentrope e(z) from isentropic relation de = -P dv.



Analysis: History of the Inverse Problem

• The forward "cylindrical bomb" problem was analyzed by G.I. Taylor in 1941. He further noted that the problem could be inverted to extract EOS information...

"The analysis here given opens up the possibility of using a tube of detonating explosive to investigate the pressure-volume relationship in the expanding gases. It is clear that either a rotating mirror photograph or a spark photograph would give the shape of the expanding case, and if this shape could be accurately determined, and if the detonation velocity had been measured, the pressure distribution in the expanding case could be measured... It seems unlikely that it would be possible to determine the shape of the expanding case with sufficient accuracy to ensure anything but the roughest estimates of the adiabatic p, v relationship."

- Taylor expressed concern about measurement error, but with modern instruments that is not the chief problem, but rather the simplifying assumptions of the model.
- There was no use for an accurate EOS in Taylor's day, because there were no computers. Nor could he have inferred an accurate EOS at that time, because the model manipulations (though quasi-analytic) are complicated in detail. But the method is ideal for symbolic manipulation programs such as *Mathematica*.

Analysis: Status of Taylor's Method Implementation

Pure Model (circa 1996)

- Has many desirable features, but expansion energy is ~10% low. This strong feature could not be corrected by geometric refinement, or even the more ideal Sandwich test.
- Problem appears to be a small but cumulative error in the volume integration step, due to a breakdown in the ideal assumptions at high pressures.

Empirical Correction

• Desire a simple empirical, but physically-motivated, correction. A successful strategy has been to adjust the magnitude of the high-pressure term in the volume ODE proportionally to the jump-off angle, which characterizes the severity of the non-ideality.

Other Refinements Since Original 1996 Model

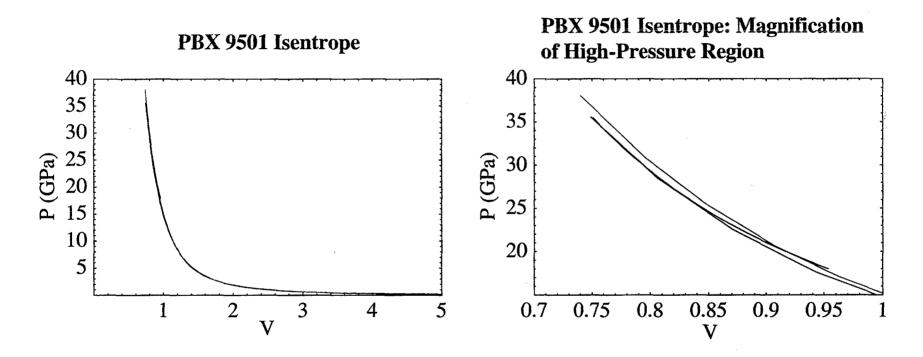
- Detonation pressure constrained to enforce c-j tangency. (Improves P_{cj} prediction while enforcing a thermodynamic constraint).
- Cylinder wall-strength included (a modest correction at low pressure).

Validation

• Model is in "beta" testing, but has passed many stringent tests (examples to follow). Validation will move to hydrotesting phase with the help of Holmann Brand (X-7)

PBX 9501 Standard: Results in *P-V* Plane

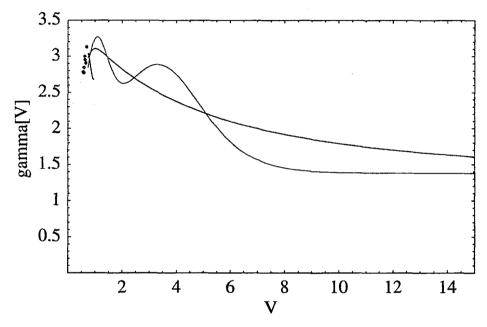
• Results for my implementation of Taylor/Hill method (black), a published JWL (red), and Sam Shaw's calculation of 1D tests (blue).



• Taylor/Hill and Shaw curves agree with each other almost exactly, over about 2/3's of Shaw's range. Shaw's curve moves toward JWL in the last 1/3 of his range.

PBX 9501 Standard: Results in γ -V Plane

• Results for Taylor/Hill (black), a published JWL (red), Shaw's calculation of 1D tests (blue), and Fritz et al.'s overdriven points (green).

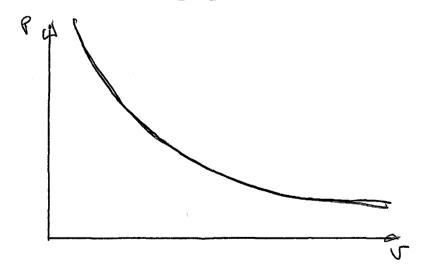


- Taylor/Hill: has the expected features: 1) lines up with Fritz points, 2) single peak at $\sim V = 1$, 3) expected c-j point, 4) correct total energy, and 5) expected ideal gas limit.
- JWL: all over the place. This is an aberration of the form.
- Shaw: drops rather steeply from c-j. Would have to take a sharp turn to the right just past the data region, to maintain the right energy.

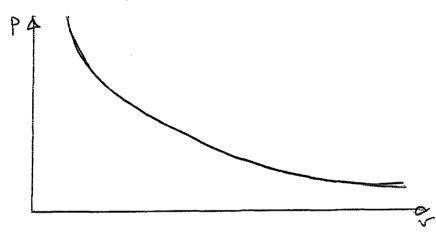
Analysis: Validation Examples

- Wish to test generality of the empirical correction for non-zero jump-off angle.
- Preliminary validation has to do with global similarity to JWL P-v isentropes: we know that JWL is pretty good in the P-v plane overall...

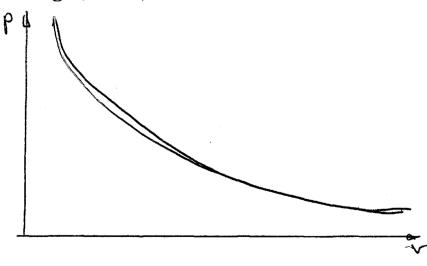
Non-standard proportions (1/2-wall) test



Standard Test; Non-Ideal HE (PBX 9502)



Large (4-inch) test + Non-ideal HE (ANFO)



Analysis: Gruneisen Gamma from Differing Initial Densities

• Taylor's method give's principal isentrope:

$$v, p_s[v], e_s[v] \rightarrow p_s = fn[e_s, v]$$

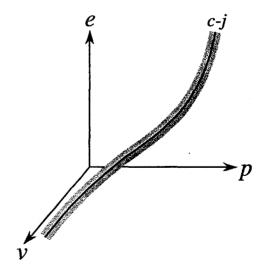
• To compute states off the principal isentrope (e.g. re-shock problem) one must know a portion of the EOS *surface*. One may consider a perturbation off the principal isentrope, given by the Mie-Gruneisen form, where $\Gamma[v]$ is "Gruneisen" gamma:

$$p - p_s[v] = \frac{\Gamma[v]}{v} \left(e - e_s[v] \right) \quad \text{where} \quad \Gamma[v] = -\left(\frac{\partial \ln[T]}{\partial \ln[v]} \right)_s = v \left(\frac{\partial p}{\partial e} \right)_v$$

- Knowing $\Gamma[v]$ on the isentrope defines the EOS in a narrow strip off the isentrope...
- From a second test at a lower density one may estimate $\Gamma[\nu]$ from the two different isentropes:

$$\Gamma[v] = v \left(\frac{\partial p}{\partial e} \right)_{v} \approx v \left(\frac{p_{2}[v] - p_{1}[v]}{e_{2}[v] - e_{1}[v]} \right)$$

• First attempt was not too successful, but there were known data problems. Will re-test soon.



EOS Forms: JWL

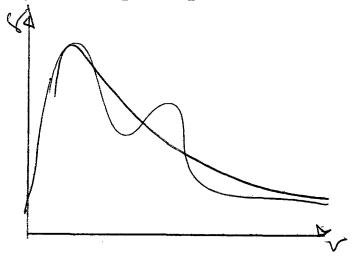
- Calibration: Using Taylor's method, JWL calibration becomes a pure least squares problem with constraints. There is no fuss and reduced ambiguity.
- Constraints: 1) V_{cj} related to P_{cj} through Rayleigh line: isentrope must pass through both, 2) c-j tangency, 3) total energy, 4) ideal gas gamma. Free parameters: R_1 and R_2 .
- Comments on JWL...

Beware: A large minority of the JWL parameters in the literature are not thermodynamically consistent. This can lead to BIG hydrocode problems.

Global accuracy is achieved by a proliferation of terms and parameters (analogy: polynomial least-squares) Try differentiating!!

Claims of JWL accuracy may often be because the calibration is well-tuned to the calculated regime. But JWL will not be accurate everywhere. Push the error down one place, and it pops up another.

JWL isentrope is a bit crazy in the γ ("sound speed") plane...



Example: JWL isentropes are too energetic for V >~ 5 if the physical value of gig is used. A better fit is obtained to V ~ 10 if an artificially high γ_{ig} is used. But $\omega = \gamma_{ig}$ - 1 determines off-isentrope behavior for JWL, which is a different consideration.

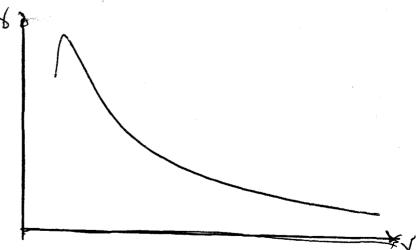
EOS Forms: Custom Formulated-Analytic Equations

- Strategy: Need analytic expression for internal energy (W. Davis). Then all other expressions can be generated analytically via it's derivatives. (Accurate expressions for $\gamma[V]$ or P[V] generally cannot be integrated.)
- Example: PBX 9501 data of Fritz et al. suggests that $\gamma[V]$ is essentially linear above c-j, over a wide pressure range (simplest non-trivial expression for $\gamma[V]$). This gives the following isentrope, for which the energy is a special function...

$$\mathcal{E}(v) = A+bv \qquad b=b^{-1}(\sqrt{c})^{-1} \qquad \qquad \mathcal{E}(v-v^{-1})$$

$$\mathcal{E}(v) = -\frac{1}{2}(v-v^{-1})$$

• Example of an expression for internal energy that fits my numerical isentropes extremely well, and which has a good $\gamma[V]$ behavior far above c-j...



Future Directions for Product EOS Effort

FY01...

- PBX 9501 Sandwich Test (1 ea.): Repeat of low density test (shot# 666) that had instrumentation problems (for Gruneisen gamma)
- PBX 9502 Sandwich Test (2 ea.): Width convergence study, EOS analysis, front curvature for DSD boundary conditions.

FY02...

- Cylinder tests on various materials -> for R. Flesner
- Modified Sandwich tests to further examine DSD boundary conditions -> for X-4
- Optimal VISAR probe design for cylinder and sandwich tests (minimize 2D effects)